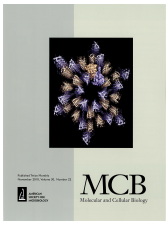
NIGMS East Coast Structural Biology Research Facility

http://protein.nsls.bnl.gov

Science Advisory Committee meeting

14 February 2011

Vivian Stojanoff
for the X6A team



Our Mission

Provide first class resources to the biological- biochemical-, and biophysics- communities to explore all aspects of structural biology. It is the goal of this facility to provide assistance to expert and non-expert crystallographers.

This goal includes:

- Beam line access to a structural biology community at large.
- Fast access to beam time for the user community.
- Crystal screening and high-throughput data collection.
- Assistance and training for academic and professional users.

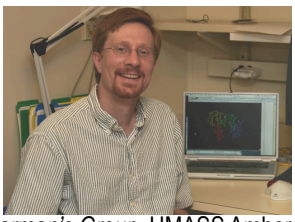
NIGMS metrics review requirement

X6A NSLS NIGMS

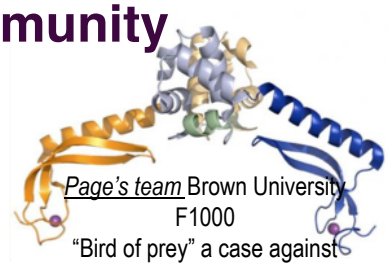
- Scientific Productivity
  - user number
  - quality of science
  - comparison with similar beam lines
- User satisfaction
- Beamline performance
- Technical and infrastructure development
  - quality
  - importance
  - relevance to user program
- Resource allocation
- Interaction with other programs at the NSLS
- Future plan

A dynamic user community

Rodrigues-Romero's Group, UNAM
Lambda6 light-chain fibrillogenesis
J Mol. Biol.

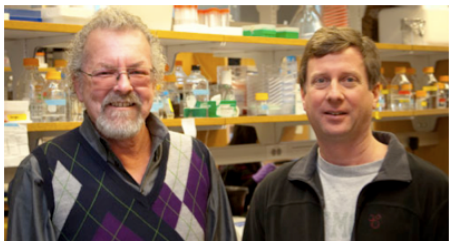


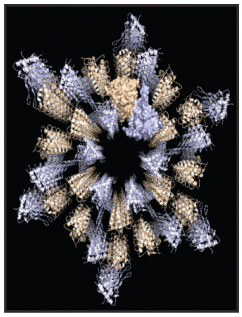
Garman's Group, UMASS Amherst,
Human Lysosomal enzymes
J Biol. Chem.
F1000 recommended



Page's team Brown University
F1000
"Bird of prey" a case against drug-resistant biofilms;
J Biol. Chem.

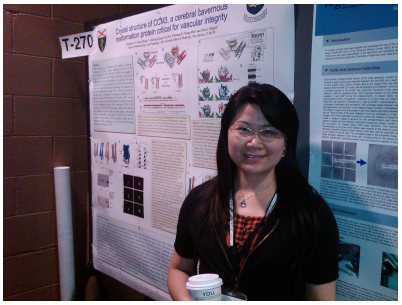
Kull 's Group, Dartmouth College
How does Cholera bacteria become infectious?
PNAS





Skordalake's team, Wistar
Telomere length regulation
Mol. Cell. Biol.

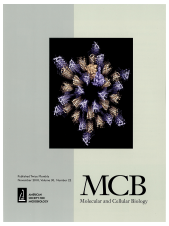
Boggon's Lab, Yale University
CCM3, a cerebral cavernous malformation protein critical for vascular integrity
J Biol. Chem.



A productive user community

67 Publications in 2010 with 20 in premier journals.

<IMPACT>= 6.5



Huang	***Nature** 464:1062-1066*
Aggarwal	***Nature** 465:1039-1043*
Miller	***Nature** 468:844-847*
Schlessinger	***Mol Cells.** 29:443-448*
Peti	***Nat.Struct.Mol.Biol**. 17:459-464*
Skordalakes	***Nat.Struct.Mol.Biol**17:513-518*
Kong	***Nat.Struct.Mol.Biol** 17:955-961*
Amzel	***Plant Cell.** 22:2970-80*
Kull	***Proc Natl Acad Sci U S** 107:2860-2865*
Schlessinger	***Proc Natl Acad Sci U S** 107:2866-2871*
Hoelz	***Proc Natl Acad Sci U S** 107:10406-10411*
Klein	***Proc Natl Acad Sci U S** 107:15075-15080*
Zhou	***Proc Natl Acad Sci U S** 107:18433-18438*
Li	***EMBO J.** 29:2037-2047*
Meruelo	***Cell Death Dis.** 1. pii: e42*
Seeman	***J Am Chem Soc**. 132:15471-15473*
Amzel	***J.Am.Chem.Soc**. 132:15565-15572*
Skordalakes	***Hum Mol Genet.** 19:1033-47*
Skordalakes	***Aging** 2:731-734*
Skordalakes	***Mol. Cell Biol**. 30:5325-34*

Outline

- Background
- Resources
- Staffing
- User Program
- Productivity
- Education and outreach
- Synergy
- Summary

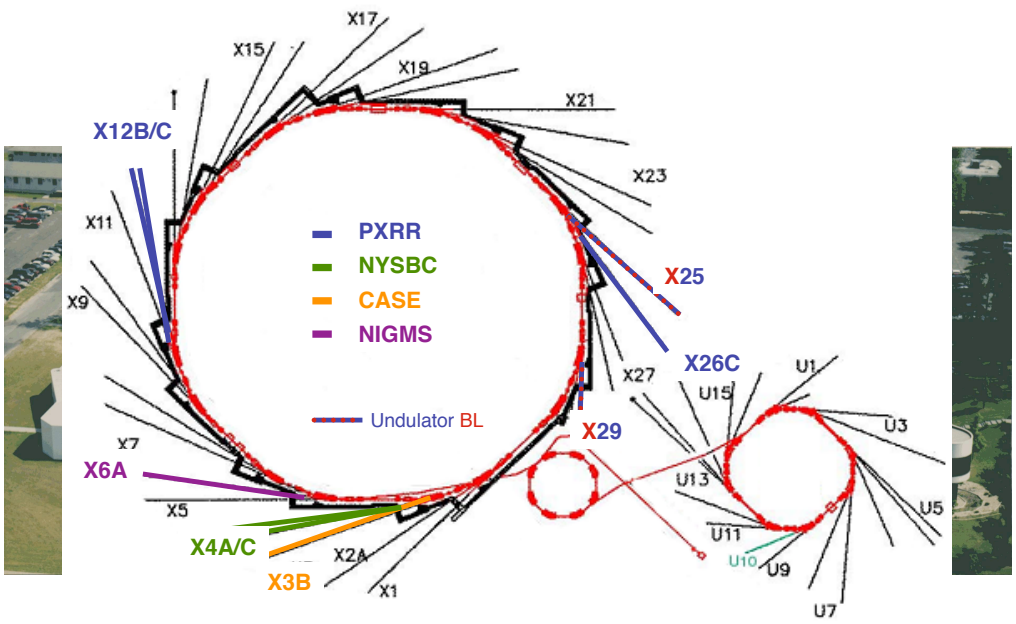
Background

The 1999 NIGMS Initiative at the NSLS

Bending magnet source recommended by NIGMS

- 2000 procurement slits, mirror, detector
- 2001 construction and installation, monochromator NSLS design
- 2001, two FTE's hired for operation support
- X6A program includes support for four FTE's
- 2002 operation start
- 2003 $1,200K supplement for detector upgrade
- 2008 End-station upgrade (November, 2008)
- 2009 End-station commissioned (March 2009)

MX at the NSLS



Resources

Optics

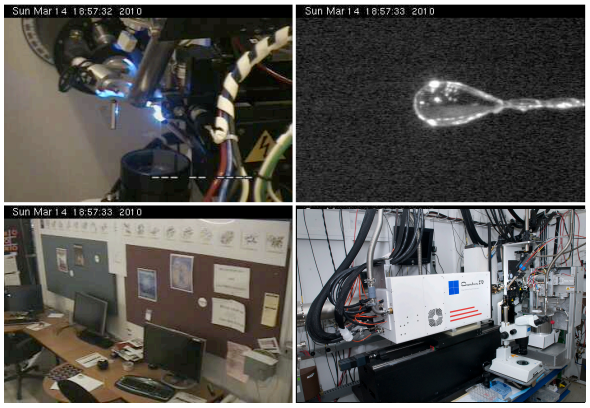
Standard optics design: current operation mode 7 to 16 KeV

Optical element				
	crystal channel cut	*energy range*	*band pass*	*Total Flux*
monochromator	Si(111)	6 -23 KeV	1.9×10^{-4}	1.2×10^{12} ph/s
	coating	figure	magnification	acceptance
mirror	Rh	Thoroidal	1:1	3mrad

* I=260 mA, 10KeV

Experimental Environment

In the Q270 first year of operation it became clear that the storage capability needs to be upgraded



	Configuration after the 2008 upgrade
Data collection Beamline control	4 x 2.2 GHz CPUs 4 Gb RAM GiBit Network 1 TB RAID 10
Data processing Storage	4 x 2.8 GHz CPUs 4 Gb RAM GiBit Network 1 TB RAID 10
	4 x 3 GHz CPUs 4 Gb RAM GiBit Network 3.6 TB RAID 10
Storage	Inhouse Storage GiBit Network 1.8 TB RAID 1

The X6A Web and Data Base Environment

Media Wiki

- Improve communication

User and Experimental Control Databases

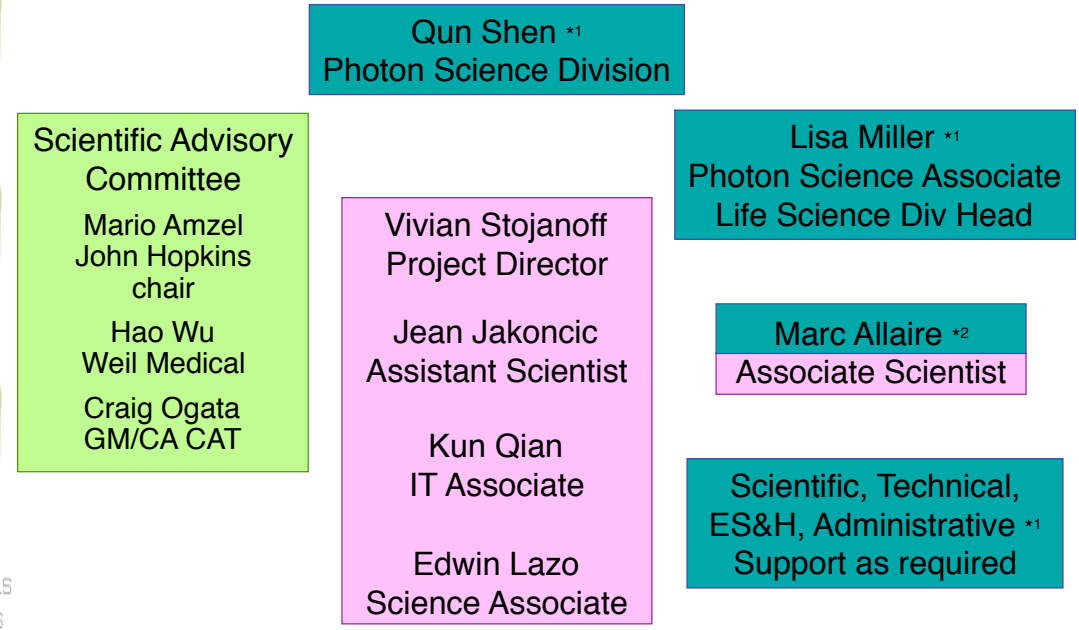
- Communication between databases

User Database

- Improve User Access
- Improve Beam Line Management
- Real time Statistical Analysis of beam time usage

Staff

Organizational Chart



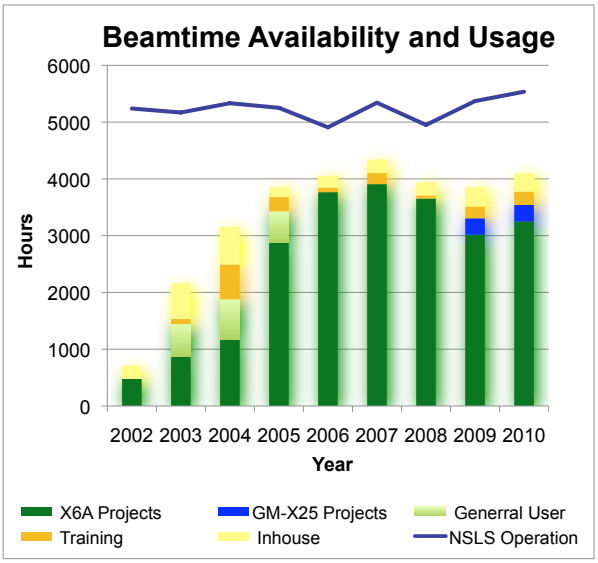
*1 PS Directorate scientific staff

*2 1/4 FTE

Beam time usage

Available beam time

Approximately 68% of the NSLS user available beam time at the GM Facility was used by researchers visiting or accessing the Facility



Beam time Utilization

X6A Program 2010

- X6A user projects 65%
- Available 9%
- X6A beam line 26%
  - ✓X6A commissioning 74%
    - ✧Instrumentation, methods development, upgrade
    - ✧Instrumentation failure (cryosystem, detector cooling system…)
  - ✓X6A inhouse projects 20%
    - ✧Scientific staff research
    - ✧Training – students in summer program

User beam time usage

Total # images	359571
Total # images screened	19714
Total#data sets*	933
Total # crystals screened and collected	6095
Automated Sample Changer	
Total #images screened	4218
Total # data sets*	40
Total # crystals screened and collected	1466
usage	27d 2 h

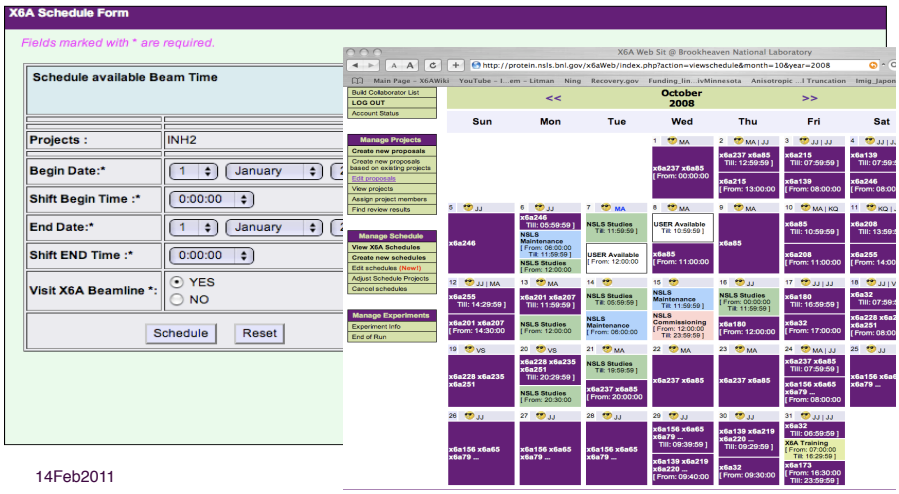
*data set 40 or more images

User Program

…"so far there might be some new great results. Thanks for your continuous support"…

Self scheduling

Unique amongst MX beam lines world wide the beam time self-scheduling function, a preferred feature between users, has been extended to offer beam time on the NSLS insertion device beam line X25.



On site users

Most of the X6A projects are carried out by users who visit the facility

- Groups are in average composed of 2-3 individuals
- Average experiments are 1.5 days
- Most leave with an electron density map

Automounter demand is increasing steadly

- 27 days scheduled
- 1466 samples were screened
- 40 data sets collected

Off-site users

User group need to have visited at least once .

ProteinXpress* — Your protein structure one shipment away

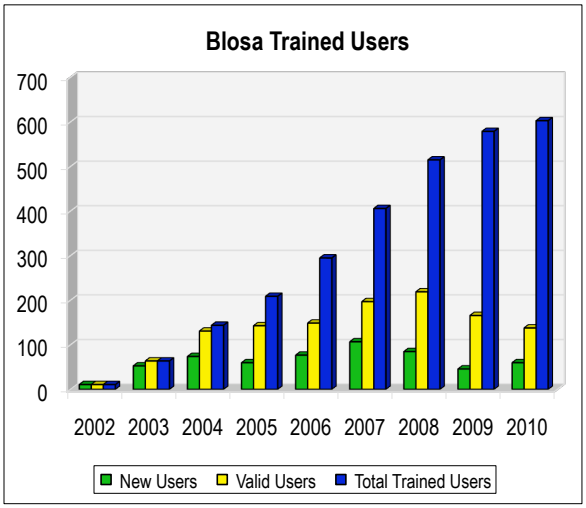
- User leaves behind or MAIL their samples
- Receive image files and scaled data
- Receive an electron density map

Remote Users

- User controls the end-station and data reduction from home Institution;
- Access through NoMachine; requires BNL VPN account;
- Lots of interest;
- Needs to be streamlined

* Is the preferred mode by off-site users

BLOSA (Beam Line Operation and Safety Awareness) trained users*

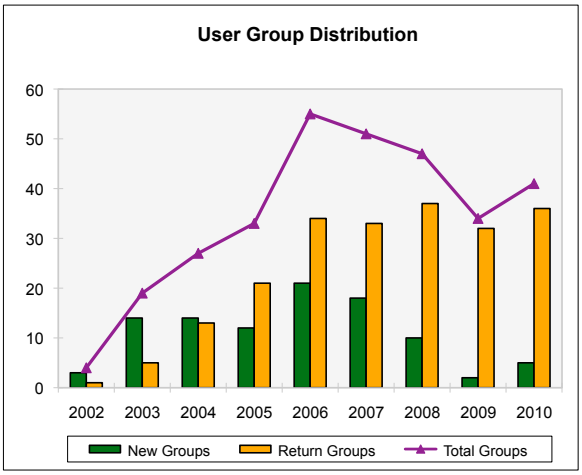


*Source NSLS PASS System December 2010

BLOSA training is valid for two years.

**New Users*: are experimenters who got trained in a specific year and were never BLOSA trained in previous years.
**Valid Users*: are experimenters who keep a valid BLOSA Training Status in a specific year.
**Total Trained Users*: are experimenters who trained in that year or before (accumulated number). Numbers include new and returning users.

Consolidation of the user community*



New groups: scheduled their projects only once in 2010.

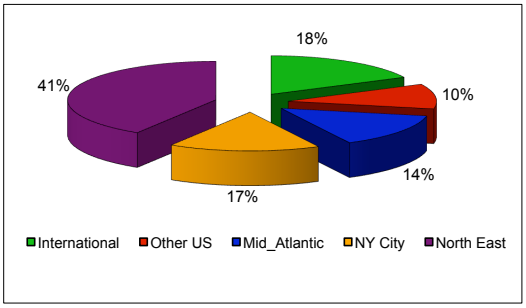
Return groups: scheduled their projects at least 2x in 2010.

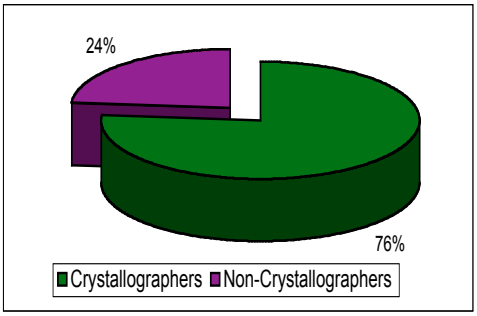
*Source X6A Survey December 2010

The number of user groups returning to the beam line is approximately constant with a 6% fluctuation over the past years. A slight increase in new user groups is observed in 2010.

User demographics*

The number of user groups from academic institutions visiting the beam line remained approximately constant; slight shifts were observed between groups.

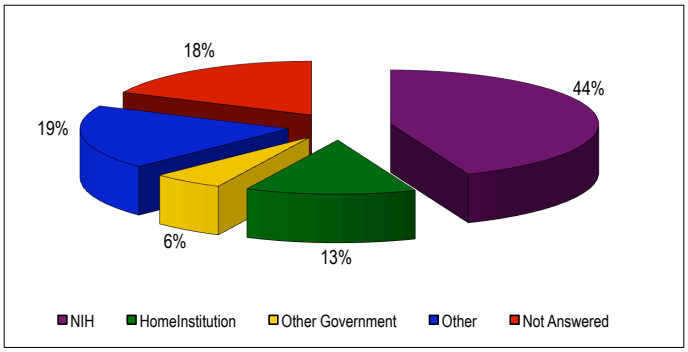




*X6A survey Dec2010

The number of non-expert users fluctuates. Less then 54% of the users provide this information when registering as X6A member. Further more most non-crystallographers do not register on the X6A webpages.

User Funding Sources*

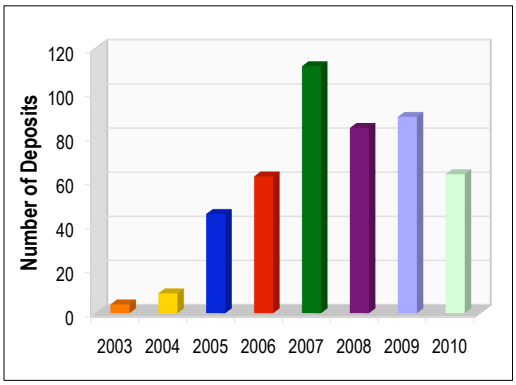


The number of user groups receiving funding from one of the NIH Institutes and Home Institutions increased by 2% in 2010. Contributions from other funding sources remained constant.

*Data X6A survey Dec2010

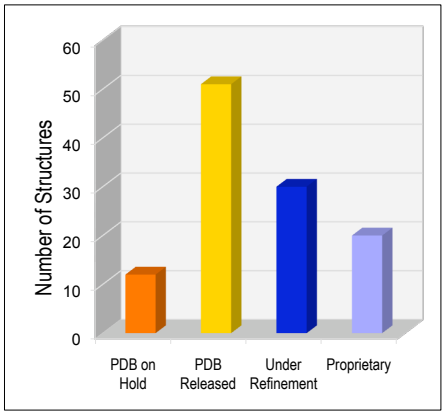
Impact

Protein Data Bank Deposits*



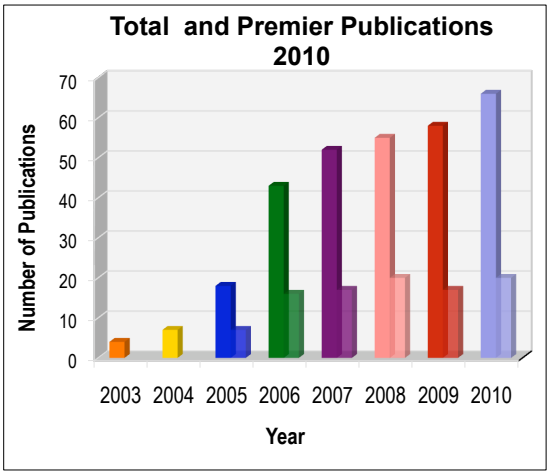
Number of deposits (released and on hold) is leveling off at about 60 per year.

The number of structures deposited in the PDB is not complete. Each year a few new releases are captured for past years as far as 5 years back.



*Source X6A Survey December 2010

Publications*



Publications*	
Total	High Impact**
303	97
2010	
66	20

*Source X6A Survey December 2010

** Journals with an impact of 6.0 or greater. Source JCR 2007

In spite off a thorough survey the total number of publications in a given year are not completely captured. An overall increase in publication numbers was observed for the last three years. As expected for a maturing beam line the number of publications/year seems to be leveling off.

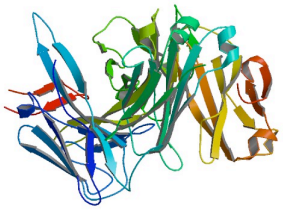
Publications 2010 - Highlights

In 2010 our user community was very productive with 67 publications, 20 in premier journals. The average impact factor is:

<Impact> = 6.5

Projects developed by the user community

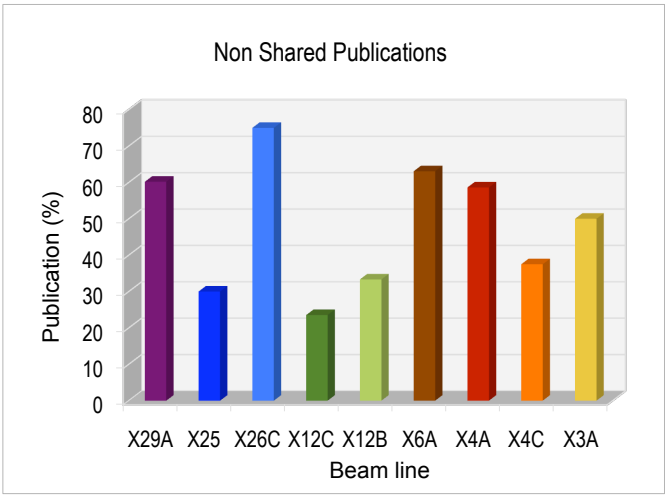
- were recommended by Faculty of 1000
- appeared in editorials
- subject broad impact media



Nat.Struct.Mol.Biol. 17: 955-961 (KONG)

Publications shared with other NSLS BL*

The X6A community is very active and loyal

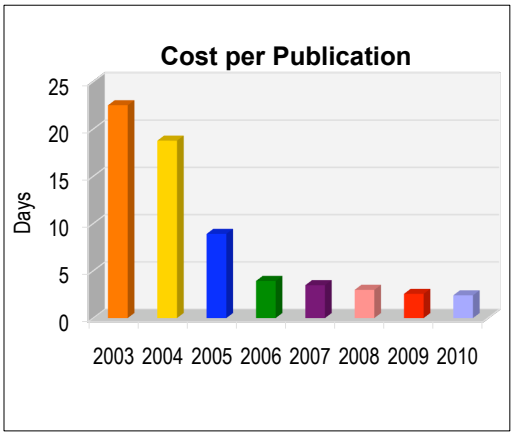


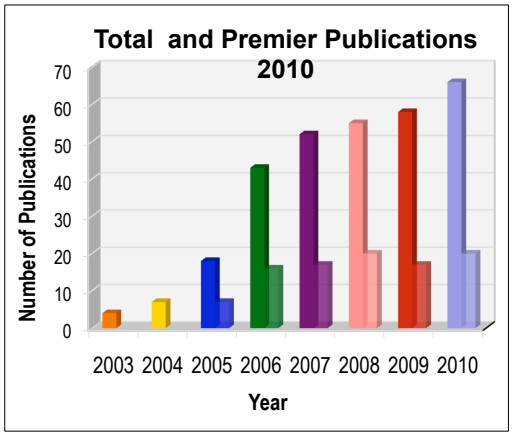
According to the NSLS publication survey approximately 63% of the X6A publications are not shared with other Facilities; ~27% of the publications are shared with NSLS insertion device beam lines, X29 and or X25.

*Source NSLS website 2010

Other impact factors*

It is common to refer to the cost per structure, per paper…..





The cost per paper per structure as a function of scheduled user hours leveled off.

NSLS
NIGMS

Education and Outreach

… the 2010 Spring workbench greatly helped me in my project.

NSLS
NIGMS

Education and outreach

X6A team members and interns participate in courses and workshops. This is an important activity to attract new users.

- Workbench
- DOE summer internship program
- NSLS Summer Sunday
- CCNY Summer Program
- Graduate Course

The X6A Workbench, June 10

Synergy

Synergy

The X6A team continues to make the facility available to user groups from other communities and promotes complementary methods between its user community. In specific:

- X4 PRT
  - User beam time re-allocation
  - Technical and scientific approaches to crystallography
  - Educational outreach (X6A Workbench)
- PXRR
  - Hardware support; the Q210 was lent to the PXRR for continued operation of beam line X26C

Summary

- FOCUS on the USER.
- Young Faculty User base.
- USER RESEARCH program ALIGNED with NIGMS Road Map
- One of the most productive beam lines at the NSLS.
- Continued upgrade of instrumentation assures optimal beam time usage.